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# Design of Efficient, Stable and Lead Free Perovskite Solar Cells

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## 1.0 Introduction

- The past 10 years have witnessed exciting developments in the field of Perovskite Solar Cells (PSCs). Recent research publications in the field have reported on high efficiency devices demonstrating a power conversion efficiency of around 25.5% certified by the NREL. This by far exceeds the efficiency of most silicon based solar cells sitting between 12 to 16%. Furthermore, the fact that PSCs can be produced via less complex solution processing methods using a variety of abundant, readily available raw materials makes this technology very promising as the future for both commercial and domestics solar energy harvesting technology. However a number of outstanding issues remain to be addressed before practical commercial PSCs can be launched into the market. The major challenge is that PSCs developed to date have poor stability that limits their operational life to just 10000HRS under simulated laboratory conditions at 0% loss in efficiency, which by far falls short of the 20 years plus, silicon solar cells can operate under real world conditions. The Second challenge is that the highly efficient PSCs are made based on perovskite films that contain toxic lead that can easily degrade under environmental stressing which makes them easily become an environmental hazard. In this current work our studies are aimed at developing improved perovskite films that are less susceptible to degradation under environmental stressing and that do not contain toxic lead. Studies conducted so far point towards a solution where we can apply computational modelling to screen materials that can alternatively substitute Pb while maintaining comparable structural consistency that does not diminish the high level of efficiency that have already been achieved. Also theoretical studies done so far point towards reduced dimensional perovskite structure as a possible solution to some of the stability challenges that are associated with

## 2.0 The low cost Solution Processing Method for Making Perovskite Solar Cells

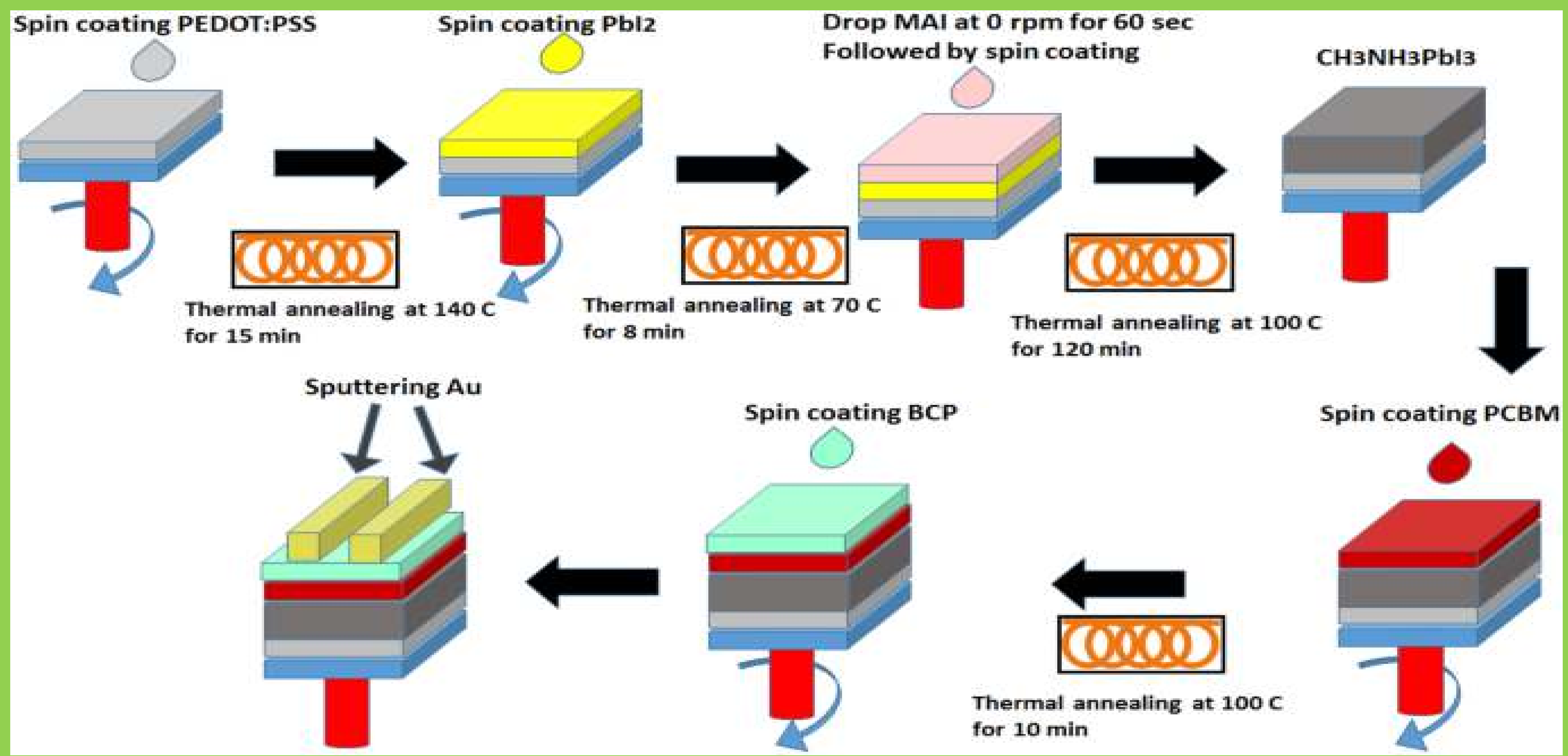


**Figure 1: Solution Processing of Perovskite Solar Cells**

## 3.0 Theoretical Framework

One advantage of PSCs is that perovskite film can be made from a diverse range of elements in the periodic table. Our work is premised on principles of crystalline solid state materials, where it is understood that crystalline material have a periodic orderly arrangement of particle of the constituent components making up the solid. Perovskite crystals have a parent 3D structure that can be described as a network of corner sharing $BX_6$ octahedra with a general $ABX_3$ stoichiometry as illustrated in figure 2. This structure is broadly responsible for the properties and characteristics exhibited by perovskites. Key factors affecting this structure are ionic radius, ionic valence and the coordination type of A, B and X ions. The variation of these aspects of the structure of perovskite constitutes the underlying framework upon which improvements can be made to address the various challenges that need to be addressed to make perovskite toxic lead free and last longer in operation at high efficiencies.

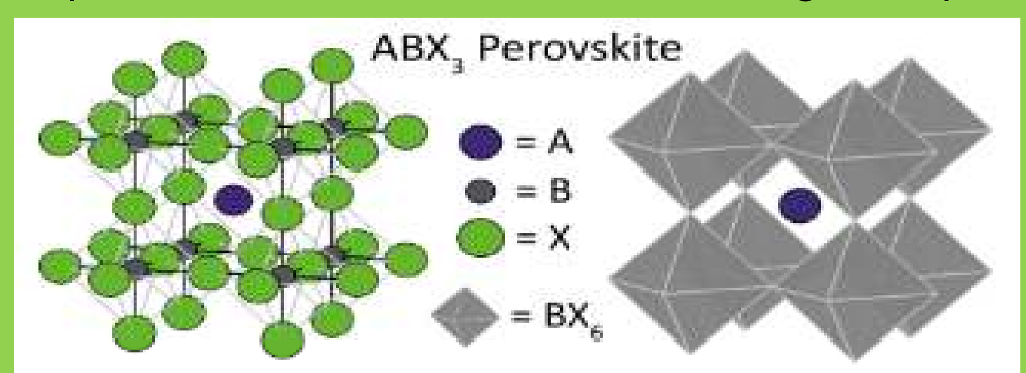


**Figure 2: Parent 3D Structure of Perovskites**

## 4.0 Methodology

Our approach is to first formulate our perovskite materials using theoretical methods mainly DFT and ab intio in the computer environment that enables us to perform an extensive search of materials that can best meet our design objectives. A number of open licence software tools are available for use in this context including VASP, Ab Init and Quantum Expresso. Our hypothesis in this context would be to prove that chiral perovskites can actually be used to design high efficiency perovskite solar cells compared to non chiral 3D perovskites. We intend to induce chirality in our perovskites by method of incorporating large chiral organic ligands in-between layers of 3D perovskites to produce layered halide perovskite films at a nano scale.

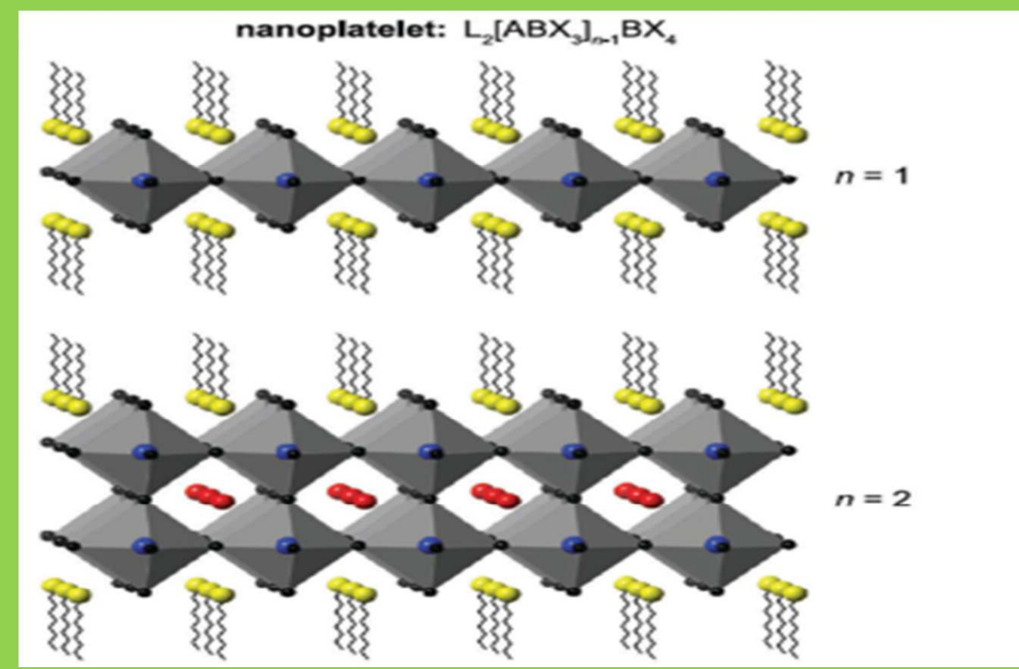


**Figure 3: Illustration of chiral perovskite**

Secondly based on the results from the computational modelling procedures, perovskite solar cells based on chiral perovskite film will be fabricated at laboratory scale via solution processing and vapour deposition techniques, then subjected to testing for proof of concept and characterisation of devices.

## 5.0 Expected Outcomes of the Research

On completion of this work we expect to:-

1) Have a formulation for making practical chiral perovskites for application in Perovskite Solar Cells.

2) Demonstrate high efficiency, stable lead free Perovskite Solar.

3) Fabricate prototype Perovskite Solar modules based on perovskite solar cells developed in this projects.

**Figure 4: General appearance of PSCs after laboratory Scale Fabrication**

## References

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